

# Snakemake

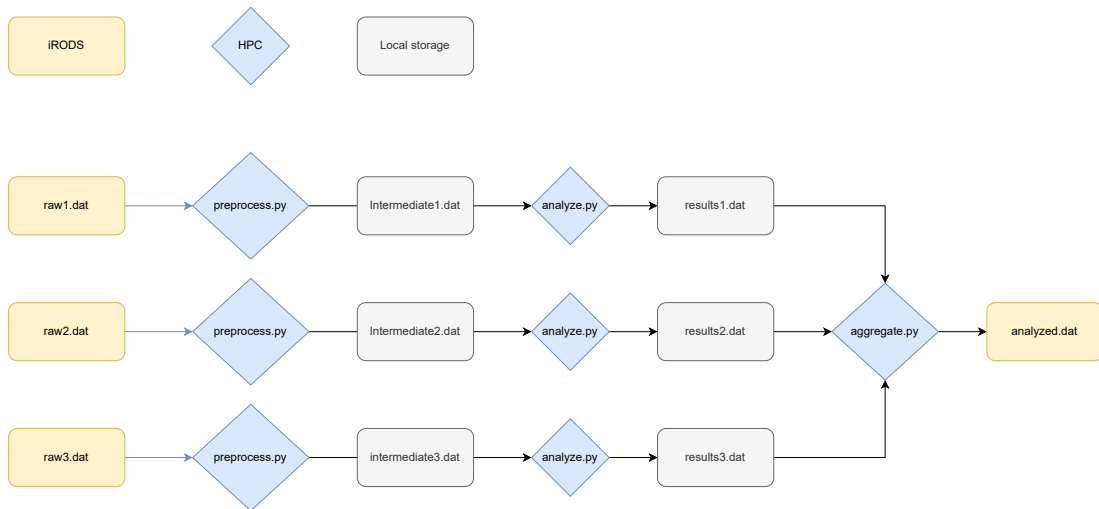
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# What is a computational workflow?



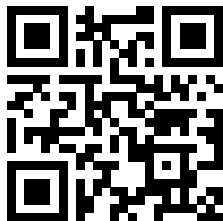
# What is Snakemake?

- Workflow engine from 2012 (Paper) inspired by Make
- More than 10 citations a week
- Active development
- Open Source, MIT
- Install through conda
- “Syntactical extension of Python”
- Steps through input and output files
- Support for different execution backends (SLURM) and remote storage (S3)
- Dynamic workflows (checkpoints)

```
rule myrule:
    input:
        "path/to/inputfile",
        "path/to/other/inputfile",
    output:
        "path/to/outputfile",
        "path/to/another/outputfile",
    shell:
        "somecommand {input} {output}"
```

# Presents from Sinterklaas (exercise)

- Sinterklaas asks his Pieten to distribute 10 million packages
- Problem: the Pieten have an authority problem
- Atom Piet: only indivisible numbers
- Professor Piet: only numbers that end with three
- Average Piet: only numbers that have an average decimal of 5
- Drunk Piet: only numbers that have repeated numbers (e.g. 11 or 22)
- Astrology Piet: No numbers that that end with nine
- Lazy Piet: Everything else



[edu.nl/4aftu](https://edu.nl/4aftu)

How big is the pile of packages in the canal?

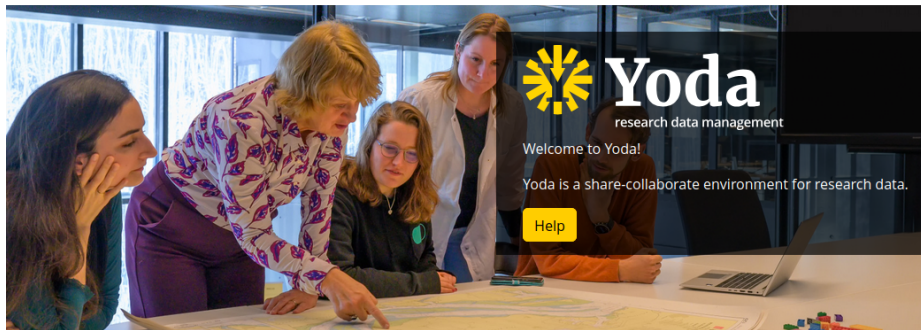
# iRODS, Yoda and iBridges

- iRODS is a datamanagement platform, at UU we have Yoda
- Not only files, but dataobjects: data + metadata
- Many ways to access it: iCommands, Yoda portal, GoCommands, iBridges



Sign in

Yoda Portal



- <https://github.com/qubixes/snakemake-storage-plugin-irods>
- Branch: `switch-to-ibridges`
- New feature: wildcards
  - Can target all files with a certain pattern
  - `/zone/user/analysis/{run_id}/temp.txt`
- New feature: metadata support
  - (iRODS) metadata is not exposed through the snakemake interface
  - `/zone/user/analysis/data.txt.metadata.json` or
  - `/zone/user/analysis.metadata.json`
  - Read or write .json files to interact with metadata
- New feature: integrate with iBridges CLI
  - Re-use cached passwords from multiple iRODS environments
- New Feature: relative paths

## Exercise part 2

- Modify the previous exercise to use an iRODS server
- `pip install git+https://github.com/qubixes/snakemake-storage-plugin-irods.git@switch-to-ibridges`
- Username/password: `test[i]`
- `irods_environment.json`:

```
{"irods_home":  "/tempZone/home/test1",  
"irods_host":  "irodserver.researchcloudde.src.surf-hosted.nl",  
"irods_port":  1247,  
"irods_user_name":  "test1",  
"irods_default_resource":  "trainingResc",  
"irods_zone_name":  "tempZone" }
```

```
1 storage:  
2   provider="irods",  
3   environment_file="/home/qubix/.irods/irods_env_surf.json",  
4   cwd="/uu/home/research-christine",  
5  
6  
7 rule all:  
8   input:  
9     meta=storage("irods://~/research-christine/test_plugin/test.txt.metadata.json")  
10
```